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U.S. DEPARTMENT OF ENERGY
PITTSBURGH ENERGY TECHNOLOGY CENTER

We have no objection from a patent standpoint to the publication or dissemination of this material

Mark P. Dvorscak

Mark Dvorscak 12-7-95
Date
Intellectual Property Law Dept.
DOE Chicago Operations Office

DIRECT COAL LIQUEFACTION BASELINE DESIGN AND SYSTEM ANALYSIS

CONTRACT NO. DEAC22 90PC89857

QUARTERLY REPORT

JULY - SEPTEMBER 1992

AMOCO

BECHTEL

JANUARY, 1993
PITTSBURGH, PENNSYLVANIA

MASTER

Bechtel

3000 Post Oak Boulevard
Houston, Texas 77056-6503
Mailing address: P.O. Box 2166
Houston, Texas 77252-2166

January 29, 1993

U. S. Department of Energy
Pittsburgh Energy Technology Center
Mail Stop 922-H
P. O. Box 10940
Pittsburgh, PA 15236

Attention: Mr. Swenam Lee
Project Manager

Subject: D.O.E. Coal Liquefaction
Base Line Design and System Analysis
Contract No. DE-AC22 90PC89857
Bechtel Job No. 20952
Quarterly Status Report
Letter No. BLD-130

Dear Mr. Lee:

Attached for your information are three copies of the subject Quarterly Status Report covering the June 22, 1992 through September 13, 1992 reporting period. Copies to other members, as required by the contract are separately and directly transmitted.

Please note that all information contained herein should be considered preliminary pending issue of the final project reports.

If you have any questions or comments on this Quarterly Status Report please contact me.

Sincerely yours,

S. K. Poddar

Syamal K. Poddar
Project Manager

Attachment

cc: Martin Byrnes, DOE/PETC
Robert Hamilton, DOE/PETC
A. B. Schachtschneider, AMOCO
File
Gilbert V. McGurl, DOE/PETC
Joanne Wastek, DOE/PETC

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1. INTRODUCTION

Effective May 16, 1990, Bechtel with Amoco as subcontractor, initiated a study to develop a computer model for a base line direct coal liquefaction design for the U.S. Department of Energy's (DOE) Pittsburgh Energy Technology Center (PETC). The project was initially for a duration of 18 months with an approved budget of $2 MM. Later, the project was extended in two steps to mid-December 1992. During this reporting period a proposal to relax the design basis for baseline by including higher space velocity for coal liquefaction reactor design basis has been granted by DOE/PETC. This is referred to as the improved baseline case and is scheduled to be completed by mid-December 1992. The study is under DOE contract No. DE-AC22 90PC89857.

The primary objective of the study is to develop a computer model for a base line direct coal liquefaction design based on two stage direct coupled catalytic reactors. This primary objective is to be accomplished by completing the following:

- A base line design based on previous DOE/PETC results from Wilsonville pilot plant and other engineering evaluations
- A cost estimate and economic analysis
- A computer model incorporating the above two steps over a wide range of capacities and selected process alternatives
- A comprehensive training program for DOE/PETC Staff to understand and use the computer model
- A thorough documentation of all underlying assumptions for baseline economics, and
- A user manual and training material which will facilitate updating of the model in the future

With the inclusion of the improved baseline case, the above primary objective is extended to include the impact of higher space velocity through liquefaction reactor.

The progress made during any particular quarter is published in a quarterly report following the duration of the quarter. The report consists of the following four sections:

- Introduction
- Summary
- Technical Progress Report (By Tasks)
- Key Personnel Staffing Report.

Introduction (Continued)

Any confidential information will be presented in the quarterly report as a separate section under the heading "confidential". As agreed upon by DOE/PETC, information included in the confidential section will be treated confidential by DOE/PETC and its contractors.

This report is Bechtel's ninth quarterly progress report and covers the period of June 22, 16, 1992 through September 13, 1992.

2. SUMMARY

Effective May 16, 1990, Bechtel initiated this study, with Amoco as subcontractor, as an assignment from the U.S. Department of Energy (DOE)'s Pittsburgh Energy Technology Center (PETC). The objective of the study is to develop a computer model for a baseline direct coal liquefaction design based on two stage direct coupled catalytic reactors. The study was for a period of 18 months which was extended later to mid-December 1992.

This is Bechtel's ninth quarterly progress report and covers the period (as requested and approved by DOE/PETC) of June 22, 1992 through September 13, 1992. This reporting period was previously covered by three already published monthly status reports.

The report contains accomplishments made during this time period in all the Tasks scheduled for the period i.e., Tasks I through VI. As per schedule, the major focus, however, was on Task II, III, IV and V. Therefore, the accomplishments included in this report are predominantly for these four tasks.

The accomplishments are presented in the report on Task by Task basis for all the Tasks covered during this reporting period.

Task I

- In Task I (which defines the project) the Project Management Plan Draft Report was completed and subsequently updated incorporating the comments and suggestions of DOE/PETC and their contractors. The final version was sent to DOE/PETC for their approval and subsequently published in August, 1990. The approved copy was the deliverable for the Task.

- Project Management Plan report covers the overall scope of work, the methodology of managing the cost and schedule of the project (configuration management), program administration, the deliverables during various phases of work and the definition of the baseline configuration.

Task II

Task II concerns the development of the baseline design as well as improved baseline design of the liquefaction complex. This task, with reference to baseline design, has been completed and the results have been published in three volumes during the quarterly progress reporting period, December 23, 1991 through June 21, 1992. Any update and results reflecting fine tuning with modeling effort will be included in the corresponding portions of the final project report.

Summary (continued)

- The design basis for the improved baseline case has been established utilizing Wilsonville pilot plant runs #257J, 261B and 261D. The improved baseline case is for a higher space velocity in the liquefaction reactors.

- The number of liquefaction reactor trains and the coal feed rate through each of the reactor trains have been finalized with the help of Amoco's kinetic model.

- The redesign of Plant 2 (Coal Liquefaction Plant) has been accomplished.

Task III

Task III concerns the development of the cost estimate and economics for the baseline design and options for the coal liquefaction facility.

- During the previous reporting period, March 16, 1992 through June 21, 1992, based on the DOE/PETC/Bechtel/Amoco review meeting of February 24-25, 1992 capital cost estimates for the baseline design as well as all seven options were completed for two different scenarios. These scenarios are for: 1) the First Plant and, 2) Nth plant. Later, the Nth plant concept has been accepted for further economic evaluation. During this reporting period, the capital cost and operating requirements for the improved baseline has been initiated.

- The comments on the draft Topical/Task III report (in 2 volumes) containing capital cost and operating requirements for the baseline and options were obtained from DOE/PETC. During this reporting period, the final version of volumes I and II of the Topical/Task report has been published. Besides incorporation of all comments, the final report contains the updated (fine-tuned) capital costs and operating requirements for all seven options for the "First Plant" and for the "Nth Plant" scenarios.

  The remaining volume (Volume III) of this report containing economics will be completed and issued as part of the final project report after the improved baseline case is completed.

Task IV

- Task IV which concerns the development of the mathematical algorithms and models was completed. The final task report was issued the first week in October, 1991.

Task V

Task V involves developing the ASPEN process simulation model of the baseline design.

- The ASPEN computer model had been tuned to match the baseline design. Capital cost changes reflecting recommendation of the DOE/PETC/ Bechtel/Amoco February, 1992, review meeting have been integrated.

- The ASPEN based kinetic model is being tuned to match the baseline design. Testing of the model is in progress.

- Completed the final tuning of the kinetic model for the coal liquefaction reactors of Plant 2 to incorporate the recent Wilsonville data.

- The draft of the Topical/Task Report for Task V was issued to DOE/PETC for their comments. This report is in two volumes; Volume I discusses the process simulation model for the baseline design and the seven option cases, and Volume II discusses the LOTUS spreadsheet economic model and the ASPEN/SP kinetic model for coal liquefaction reactors. In addition, the report has a three part Appendix which contains listings of the complete ASPEN/SP input and Fortran files, and detailed documentation for the LOTUS spreadsheet economic model.

- The previously developed kinetic and ebullated bed hydrodynamic models were used to design liquefaction reactor for the higher space velocity case. During the reporting period, optimization of the reactor design was continued. This was to account for (1) internally treated as well as untreated gas recycle rates, (2) recycle solvent composition (3) changes in overall coal conversion and ROSE-SR organic loss and (4) revised gas and liquid yields (relative to the previous baseline design) in the first and second reactor stages. The higher space velocity design case is based on four reactor trains with a coal flowrate of 343,800 lbs of MAF coal per hour per train.

- Economics model based on Lotus 1-2-3 spreadsheets has been revised to incorporate the updated set of key assumptions based on DOE/PETC's input. Revised documentation reflecting these changes has been completed.

- During May 16, 1992 through June 21, 1992 reporting period a draft of Volume I and Appendix I of the Topical/Task report for Task 5 was completed. Volume I contained documentation for 1) the baseline design and cost estimate model for the "First Plant" case and 2) the Lotus 1-2-3 spreadsheet economic model and 3) how to use it.

Summary (continued)

Task VI

This task concerns the development of a training manual and a training course for the process simulation model.

- The draft Topical Report for Task VI (training) has been revised and issued. This revision was to reflect DOE's comments and conform to the final version of the models. In addition, this report was split into two volumes; the first volume covers the ASPEN/SP process simulation model, and the second discusses the LOTUS economic model and the kinetic model for the coal liquefaction reactors.

3. TECHNICAL PROGRESS (BY TASKS)

In order to carry out this Study efficiently, the Study has been divided in seven major tasks. Task I defines the project. Task II develops the baseline design. Task III develops the capital, operating and maintenance costs. Task IV develops the mathematical model necessary for the process computer simulation model. Task V develops and verifies the process simulation model. Task VI documents the process simulation model and training. Task VII is a level of effort task for project management, technical coordination and other miscellaneous support functions.

During this reporting period (June 22, 1992 through September 13, 1992) several accomplishments were made in Tasks II, III, IV, V and VI. These accomplishments are included in this report task by task.

3.1 TASK I

Task I defines the scope and the methodology of accomplishing the project. It sets the objectives of the project and defines the paths to accomplish those objectives.

As mentioned earlier in Section 3, Task I was completed during the first quarterly reporting period and accomplishments were documented in the Project Management Plan issued in August, 1990.

The Project Management Plan report is comprised of the following 9 sections:

- Executive Summary
- Background/Introduction
- Study Objective
- Overall Scope Of Work
- Configurational Management
- Program Administration
- Deliverables
- baseline Configuration
- Appendix/Project Procedure Booklet
  List Of Contents

The report completing Task 1 was published on time schedule. Detailed accomplishments of Task I were included in the first quarterly report (May 16, 1990 through August 19, 1990) of the project.

3.2 TASK II

Task II concerns the development of the baseline design and improved baseline design of the liquefaction facility. This part of the study includes the acquisition of process licensors information, incorporation of various processing options into the design, and developing the design of the on-site processing units and offsite facilities (including storage and loading, utilities, and waste handling).

In this task certain plants are handled as packaged plants (or blocks) with an overall heat and material balance only.

3.2.1 Status Update

The final Topical/Task report for task II is divided into three volumes. Volumes I and II contain the information on the baseline design while volume III covers the options (alternates). Volumes I and II of the report were published during the quarter of September 16, 1991 through December 22, 1991 reporting period, whereas Volume III of the report, both draft and the final version were published during December 23, 1991 through March 15, 1992 reporting period.

In addition, during this reporting period the improved baseline case has been initiated and several accomplishments were achieved. These were:

1) Setting up the design basis for the improved baseline utilizing Wilsonville pilot plant runs #257J, 261B and 261D and thereby having a higher space velocity in the liquefaction reactors,

2) completing the design of liquefaction reactors of plant 2 with the help of Amoco's kinetic model and,

3) establishing overall material balances, overall hydrogen flow distribution and overall water flow distribution.

Details on these accomplishments are included in this section.

Plant 2 (Coal Liquefaction)

The key assumptions related to design basis were developed jointly by DOE, Amoco, Bechtel, and Burns & Roe.

Design Basis, Criteria and Considerations

Coal Feed

The coal to be fed to the coal liquefaction plant is washed and dried Illinois No. 6 coal (Burning Star Mine) from Plant 1, the Coal Preparation Plant. Analysis of the basis coal is presented in Table 3.1.

Process

The process used will be close-coupled, catalytic-catalytic, two-stage coal liquefaction (H-COAL by HRI) with ashy recycle, recycle of extract from the critical solvent deashing plant, and recycle of 850°F+ to extinction.

Key Design Constraints

The primary goals for the improved baseline liquefaction reactor design were:

(1) to maximize total coal throughput using the same size ebullated-bed coal liquefaction reactors (15 ft. id and 85 ft. high) that were used in the original baseline design, and

(2) to minimize the number of operating trains (5 in the original design).

The key design constraints for the liquefaction reactors were:

- Weight of each reactor: less than 1300 short tons
- Gas velocity in each reactor: less than 0.2 ft/sec
- H2 partial pressure at the second reactor outlet: about 1940 psia
- The reactor outlet temperatures should be less than 830°F to avoid catalyst sintering. The first reactor should have a reasonably high hydrogen consumption (about 3.7 wt% MAF coal) and should be operated at a higher temperature than the second reactor. For the improved baseline design, the first reactor is operated at 810°F versus 760°F for the second reactor.

Table 3.1

Analysis of Feed Coal to Liquefaction
Illinois No. 6 (Burning Star Mine)

Proximate Analysis (wt. %, Dry Basis)	
Volatile Matter	42.2
Fixed Carbon	46.3
Ash	11.5
Ultimate Analysis (wt. %, Dry Basis)	
Carbon	71.0
Hydrogen	4.8
Sulfur	3.2
Nitrogen	1.4
Ash	11.5
Chlorine	0.1
Oxygen (by difference)	8.0
Sulfur Forms (wt. %, Dry Basis)	
Pyrite	1.0
Sulfitic	0.1
Organic	1.9
Ash Composition (wt. % oxidized)	
Phosphorus pentoxide, P_2O_5	0.2
Silica, SiO_2	49.8
Ferric Oxide, Fe_2O_3	17.6
Alumina, Al_2O_3	19.2
Titania, TiO_2	1.0
Lime, CaO	6.3
Magnesia, MgO	1.0
Sulfur Trioxide, SO_3	2.9
Potassium Oxide, K_2O	2.0
Sodium Oxide, Na_2O	0.5
Undetermined	-0.5

The above maximum reactor temperature and minimum hydrogen consumption limits affect the heat liberation rate and the total bed exotherm; which in turn, controls the maximum coal flow rate.

Overall Yields

The conditions of the coal liquefaction reactor for Wilsonville Run 257-J, the improved baseline design case, and the original baseline design case are compared in Table 3.2. For the improved baseline case, the overall coal conversion was assumed to be 92.9 wt% MAF at a coal space velocity (SV) slightly lower than that used in Wilsonville Run 257-J. This lower value reflects (a) resid extinction (0.0 wt% MAF resid yield for the improved baseline case vs. 1.2 wt% MAF for Run 257-J), and (b) a lower organics loss in the ROSE-SR unit for the improved baseline case (15.7 wt% MAF vs. 18.5 wt% MAF for Run 257-J). This improved ROSE-SR unit performance is justified since Wilsonville ROSE-SR unit performance typically improved with days of operation for a given run, and during Runs 261-F and 261-G, the ROSE-SR organics losses were about 15.6 wt% MAF. The total solvent/MAF coal ratio was assumed to be 2.26 lbs/lb (compared to 2.46 lbs/lb used for the original baseline design) with the same solvent composition as that of the original baseline design.

Table 3.2
Key Operating Conditions

	257-J	**Improved Baseline**	**Baseline**
Coal SV, lb MAF/hr/lb Cat	2.17	1.95	1.12
Temp., °F Reactor I Reactor II	 809 760	 810 760	 790 760
Catalyst addn., 1bs/ton MF each stage	3/1.5	3/1.5	3/1.5
Solvent/MAF Coal	2.25	2.26	2.46
Resid in Solvent, wt%	50	50	50

The overall liquefaction yields are compared in Table 3.3. The hydrogen consumption for the improved baseline design was increased to 6.3 wt% MAF (compared to 6.0 wt% MAF in 257-J) to account for the higher C4+ liquids production. The water yield was based on Wilsonville Runs 261-B (8.3 wt% MAF) and 261-D (9.7 wt% MAF). The above H2 consumption and water yield were verified by an overall elemental balance (Table 3.4) for the improved baseline design case.

Table 3.3 Overall Product Yields			
Yields, wt% MAF	**257-J**	**Improved Baseline**	**Baseline**
$H_2S + H_2O + CO_x + NH_3$	15.1	13.9	14.0
C1 - C3	5.4	5.5	4.8
(C4 - 350)°F (350 - 450)°F	14.5 7.1	15.8 7.3	16.9 7.5
(450 - 850)°F	44.2	48.1	46.8
C4 + liquids	65.8	71.2	71.2
Resid	1.2	0.0	0.0
Organics in ash-conc.	18.5	15.7*	16.3
H_2	(6.0)	(6.3)	(6.2)

* Run 261-F/G: 15.6%

Table 3.4 Primary Liquefaction Yield & Elemental Balance Data Improved Baseline Design Case							
Mass Balances, lb.	**Carbon**	**Hydrogen**	**Nitrogen**	**Oxygen**	**Sulfur**	**Ash**	**Total**
Input							
H2	0.00	6.30	0.00	0.00	0.00	0.00	6.30
MAF Coal	80.25	5.42	1.62	9.09	3.62	0.00	100.00
Ash	0.00	0.00	0.00	0.00	0.00	12.96	12.96
TOTAL	**80.25**	**11.72**	**1.62**	**9.09**	**3.62**	**12.96**	**119.26**
Output							
H2O	0.00	1.04	0.00	8.22	0.00	0.00	9.26
H2S	0.00	0.17	0.00	0.00	2.78	0.00	2.95
NH3	0.00	0.25	1.14	0.00	0.00	0.00	1.39
CO2	0.05	0.00	0.00	0.15	0.00	0.00	0.20
CO	0.04	0.00	0.00	0.06	0.00	0.00	0.10
CH4	1.50	0.50	0.00	0.00	0.00	0.00	2.00
C2	1.40	0.35	0.00	0.00	0.00	0.00	1.75
C3	1.43	0.32	0.00	0.00	0.00	0.00	1.75
C4	0.83	0.17	0.00	0.00	0.00	0.00	1.00
C5	0.17	0.03	0.00	0.00	0.00	0.00	0.20
C6 - 350	12.44	2.07	0.00	0.07	0.01	0.00	14.60
350 - 450	6.36	0.89	0.02	0.04	0.00	0.00	7.30
450 - 650	30.17	3.78	0.12	0.17	0.01	0.00	34.25
650 - 850	12.32	1.39	0.05	0.09	0.00	0.00	13.85
ASH-CONC.	13.54	0.75	0.28	0.29	0.83	12.96	28.66
TOTAL	**80.25**	**11.72**	**1.62**	**9.09**	**3.62**	**12.96**	**119.26**

Stage I Yields

The Stage I yields, as shown in Table 3.5, were estimated as a fraction of the overall yields. Those for the improved baseline design were based primarily on Wilsonville Runs 261-B and 261-D, since in Run 257-J, the Stage I yields were not measured because the interstage separator which recovers the Stage I products was not used. Thus, for Run 257-J, the resid yield (27.0 wt% MAF) and hydrogen consumption (3.7 wt% MAF) were assumed to be similar to those of the original baseline design.

Table 3.5 Stage I Yields: Original Baseline And Improved Baseline Designs		
Yield, Wt% MAF Coal	**Improved Baseline**	**Original Baseline**
CO	0.04	0.04
CO2	0.13	0.09
NH3	0.98	0.95
H2O	6.71	7.10
H2S	2.10	2.00
C1	0.83	0.91
C2	1.19	0.74
C3	1.37	0.85
C4	0.47	0.40
C5-350°F	4.14	8.00
350-450°F	1.67	4.90
450-650°F	6.21	7.00
650-850°F	2.51	15.20
850-1000°F	40.92	18.52
Resid	27.00	26.80
UC	7.46	10.20
H2 (Consumed)	(3.73)	(3.70)

Product Quality (API Gravity)

The API gravity of various fractions of the product yields are shown in Table 3.6.

Table 3.6 API Gravity of Various Fractions	
Fractions	**API Gravity***
IBP - 350°F	50.8
305 - 450°F	29.7
450 - 750°F	19.0
750 - 850°F	9.3
850 - 1000°F	1.0
1000^{+} °F	-10.5

* The data (except for 1000^{+} °F) are based on the average values of API gravity of respective components of Wilsonville pilot plant runs 261B and 261D.

Gas Flows

The key recycle gas (i.e., the untreated internal recycle streams, as well as the treated purified hydrogen recycle stream shown in Figure 3.1) rates and compositions are given in Table 3.7. These rates were estimated (1) to correspond to the desired second reactor outlet hydrogen partial pressure (about 1940 psia), and (2) to maintain required C1-C3 gas purge rate.

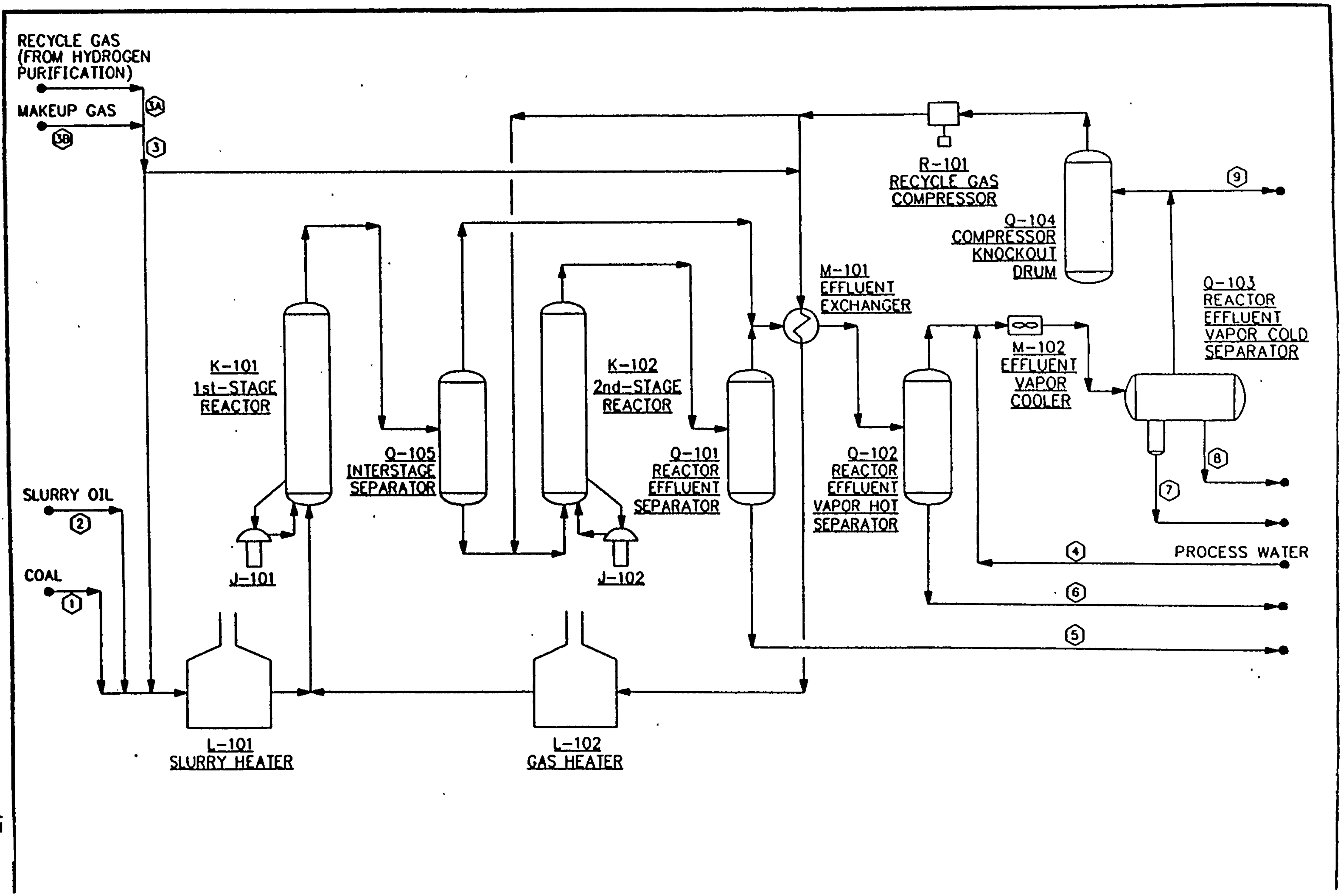
Table 3.7
Recycle Gas Flow Rates for the Improved Baseline Design

Flow Rate, lbs/hr/train	Treated Recycle Gas to Stage I	Untreated Recycle Gas to Stage I	Untreated Recycle Gas to Stage II
N_2	69	357	1433
H_2	4037	4000	16048
H_2O	13	32.7	131.3
H_2S	0	734.4	2947
NH_3	0	1.6	6.4
CO	75	390.5	1567
CO_2	0	38.9	156.1
CH_4	1366	6077	24381
C_2H_6	619	3172	12728
C_3H_8	379	1940	7784
C_4H_{10}	131	667	2678
C_5H_{12}	212	1102	4420
Total	**6901**	**18514**	**74278**

Key Design Parameters

The coal liquefaction kinetic model and the ebullated-bed fluid dynamics correlations (developed for the baseline design) were used to estimate the maximum coal feed rate per reactor train subject to the design constraints, product yields and catalyst addition rate for each reactor. Some modifications to the original USR2G Fortran kinetic model (described in Section 12 of the Topical Report for Task V) were required to account for the differences in product yields between the original baseline and the improved baseline design cases.

Figure 3.1 Key Recycle Gas
BASELINE DESIGN - SCHEME 2
BATTERY LIMITS STREAMS



As shown in Table 3.8, the space velocity assumed for the improved baseline design allowed the use of four operating trains (compared to five for the original baseline) with a 9 percent increase in overall coal throughput over the original baseline design. For the high temperature first stage, the outlet temperature was estimated to be about 827°F compared to the assumed design constraint of 830°F. Each ebullated-bed reactor has the same 15 ft internal diameter as the original baseline design, but a lower catalyst loading. For the improved baseline design, the settled catalyst bed height is about 34 ft compared to about 44 ft in the original baseline design. The ebullated-bed pump recycle rate was estimated to give a bed expansion to about 77 ft. The total gas/liquid velocities in each reactor and the hydrogen partial pressure at the second stage outlet also are within the design limits.

Table 3.8
Comparative Design Data: Baseline vs. Improved Baseline Designs

Design Cases	**Improved Baseline**		**Baseline**	
Number of Operating Trains	4		5	
Coal feed rate/train, Mlb MAF/hr	343.8		252.3	
Reactor [a,b]	**1st Stage**	**2nd Stage**	**1st Stage**	**2nd Stage**
Velocity, fps				
Gas	0.14	0.19	0.11	0.21
Liquid	0.12	0.11	0.10	0.08
Bed Height, ft.				
Settled	34	34	44	44
Expanded	77	77	77	77
Recycle/Fresh Feed ratio	5.6	3.1	6.0	3.3
Reactor Average Temp, °F	810	760	790	760
Bed Exotherm, °F	34	30	30	27
Reactor Outlet Temp, °F	827	775	805	774
H2 partial pressure, psia	2232	1934	2243	2061

(a) Catalyst: average diameter, 0.083 inches; length, 0.24 inches
(b) Reactor ID (excluding refractory), ft: 15
Refractor thickness, in.: 6
Total height, ft.: 85
Weight, Short tons: 1295

Overall Material Balance

The overall material balance for the improved baseline coal liquefaction complex is shown in Figure 3.2. The flow rates are in MLB/Hr and on dry basis unless otherwise noted. Exceptions are plants 34, 38 and 39 where material balances for these plants are shown on wet basis. To keep the figure simple, minor streams such as steam, sour water and make-up amine are not shown in this figure.

Overall Utility Balance

The overall utility balance for the improved baseline coal liquefaction complex is shown in Table 3.9. Because the utility consumptions for plants 23, 24 and 25 are small and intermittent, they are not included in this table.

Overall Hydrogen Flow Distribution

The overall hydrogen flow distribution for the entire complex is shown in Figure 3.3. This figure schematically shows the input and output flow rates in MMSCFD for several key process plants. As shown in this figure, hydrogen being produced in Plant 9 (Hydrogen Production Plant) gets distributed to Plant 2 (Coal Liquefaction Plant, the heart of the liquefaction complex) and two hydrotreaters, viz, Plant 4 (Naphtha hydrotreater) and Plant 5 (Gas Oil Hydrotreater), then as the output streams from these plants, goes through the hydrogen purification plant (Plant 6) and through the gas plant (Plant 3).

Overall Water Flow Distribution

The overall water flow distribution for the entire baseline liquefaction complex is shown in Figure 3.4. This figure schematically describes the sequence and quantity of water flow through various plants of the entire liquefaction complex. The flow rates through these plants are expressed in gallons per minute.

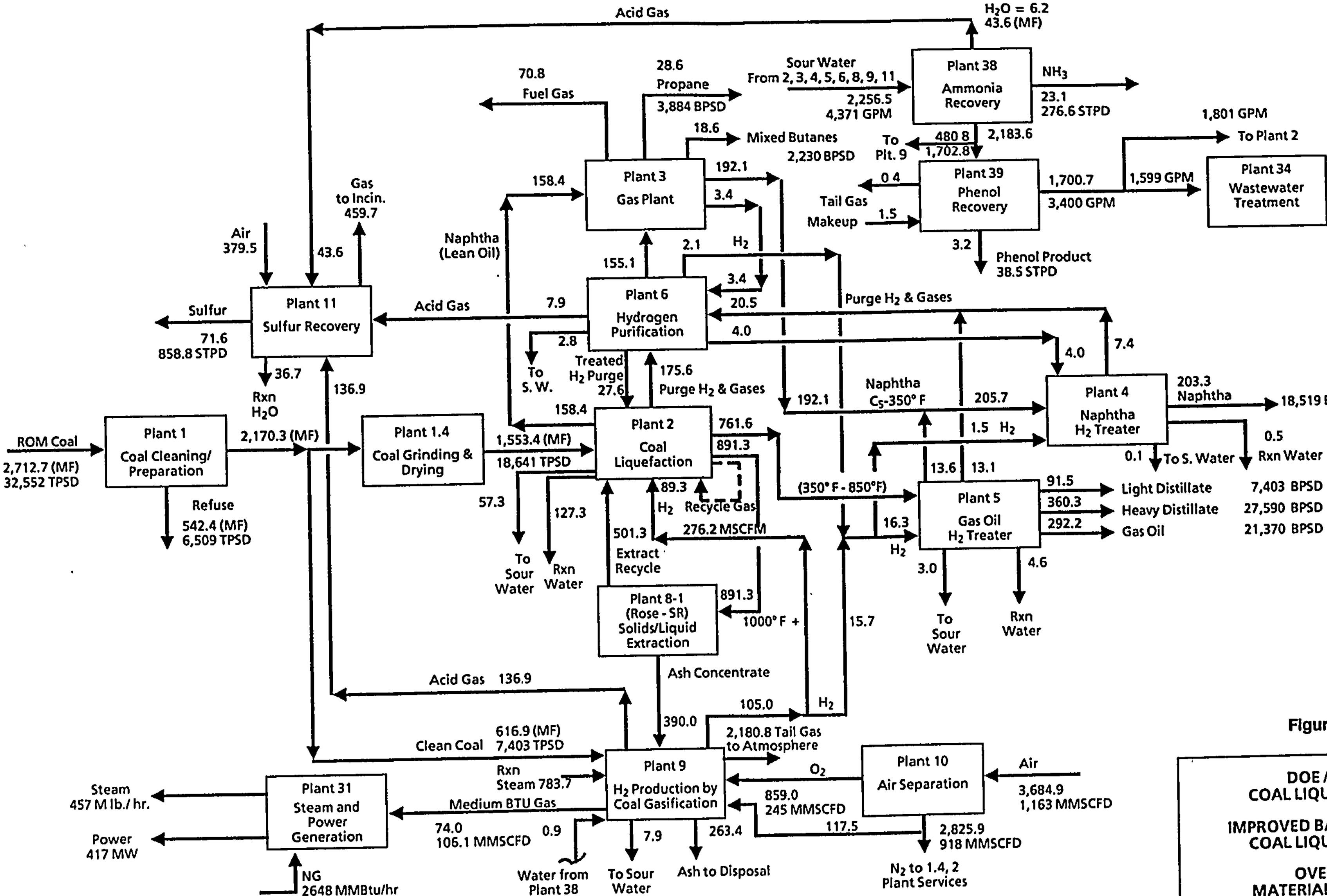


Figure 3.2

DOE / PETC COAL LIQUEFACTION

IMPROVED BASELINE CASE COAL LIQUEFACTION

OVERALL MATERIAL BALANCE

Revised 2/3/93

0992094-1

Notes:
1. Flow rates are in MLB/HR unless noted and on dry basis
2. Minor streams including steam, water, sour water, and make-up amine are not shown on this diagram
3. Flow rates around plants #38, 39, 34 are shown on wet basis

Table 3.9

OVERALL UTILITY BALANCE FOR IMPROVED BASELINE

12-Feb-93

Plant No.	PLANT NAME	Fuel Gas MMbtu/hr	Electric Power KW	Steam Psig, Lb/hr 600 Sup @720 F	600 @489 F	150 @366 F	50 @298 F	Cond/BFW Net Cons lb/hr	Cooling Water gpm	Sour Water gpm	Waste Water gpm	Makeup Water gpm	Air scfm	Nitrogen scfm
	PROCESSING UNITS													
1	Coal Cleaning and Handling		9,293								880			
1.4	Coal Grinding and Drying	530	13,204						262				6,492	81,819
2	Coal Liquefaction	1,129	59,162	6,068	(162,508)	(98,203)	176,362	462,939	8,824	(2,871)				779
3	Gas Plant	(1,504)	502		279,468		15,096	(294,564)	9,784	2				
4	Naphtha Hydrotreater	71	1,198		90,386			(90,386)	7,080	(38)		(37)		
5	Gas Oil Hydrotreater	335	2,147		62,030	(104,578)		47,548	330	(99)		(81)		
6	Hydrogen Purification		28,859			71,944	2,483	(74,427)	6,438	(101)		(84)		
8	Critical Solvent Deashing	208	4,286			24,969				(50)				
9	H2 Production by Coal Gasification	(1,112)	71,739		(331,175)	(865,844)	(886,727)	2,083,746	59,698	(1,117)	95	(1,644)		26,552
10	Air Separation		184,037											(638,630)
11	By-product Sulfur Recovery	80	3,550		69,520	(216,298)	63,157	83,621	9,422	(93)				
ALL	Common Users			73000		40000	90000	(193,000)				(532)	8508	
	Sub Total (Process)	(263)	377,977	79,068	7,721	(1,148,010)	(539,629)	2,025,477	101,838	(4,367)	975	(2,378)	15,000	(529,480)
	OFFSITES													
19	Relief and Blowdown		19											
20	Tankage		6,758			22,000	3,300	(25,300)	100					
30	Electrical Distribution													
31	Steam and Power Generation	3,760	(416,926)	(456,824)		439,435	460,436	(867,674)	69,086		(359)	(1,208)		
32	Raw, Cooling and Potable Water Systems		14,078						(263,502)		(482)	11,710		
33	Fire Protection		44											
34	Sewage & Effluent Treatment		7,313				3,000	(3,000)				(482)		
35	Instrument & Plant Air Systems		2,894										(15,000)	
36	Purge and Flush Oil System		258											
37	Solid Waste Disposal		48								90			
38	Ammonia Recovery		1,738		370,035	659,680		(1,029,715)	87,184	4,371				
39	Phenol Recovery		964			26,895	72,893	(99,788)	5,294		(1,599)			
Other	Bldg 41,42, Light, Etc.		4835											
	Natural Gas Imported	(3,497)												
	Off Site BL and Evaporation										1,375	(7,642)		
	Sub Total (Offsite)	263	(377,977)	(456,824)	370,035	1,148,010	539,629	(2,025,477)	(101,838)	4,371	(975)	2,378	(15,000)	0
											0			
	GRAND TOTAL	0	0	(377,756)	377,756	0	0	0	0	4	0	0	0	(529,480)

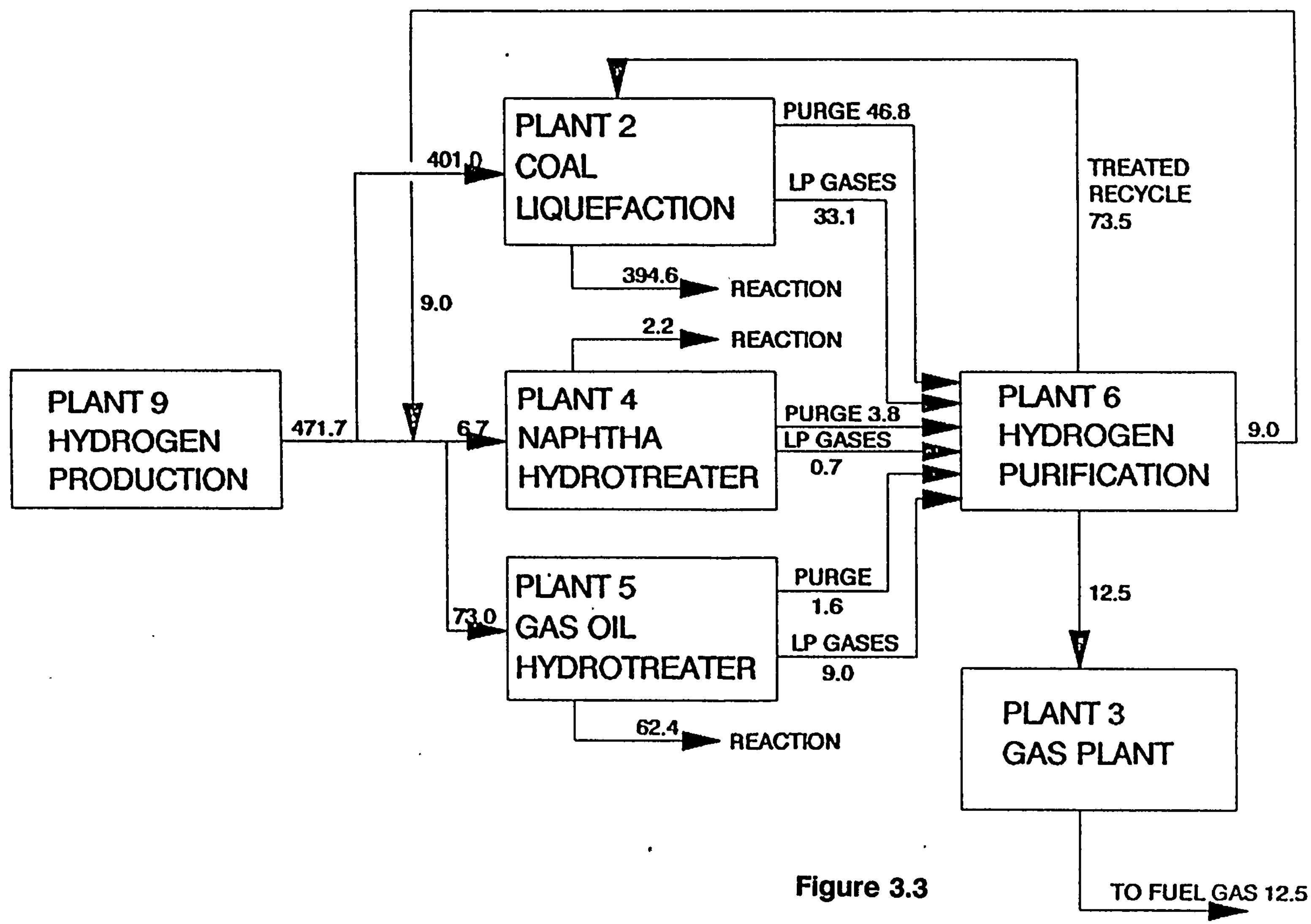
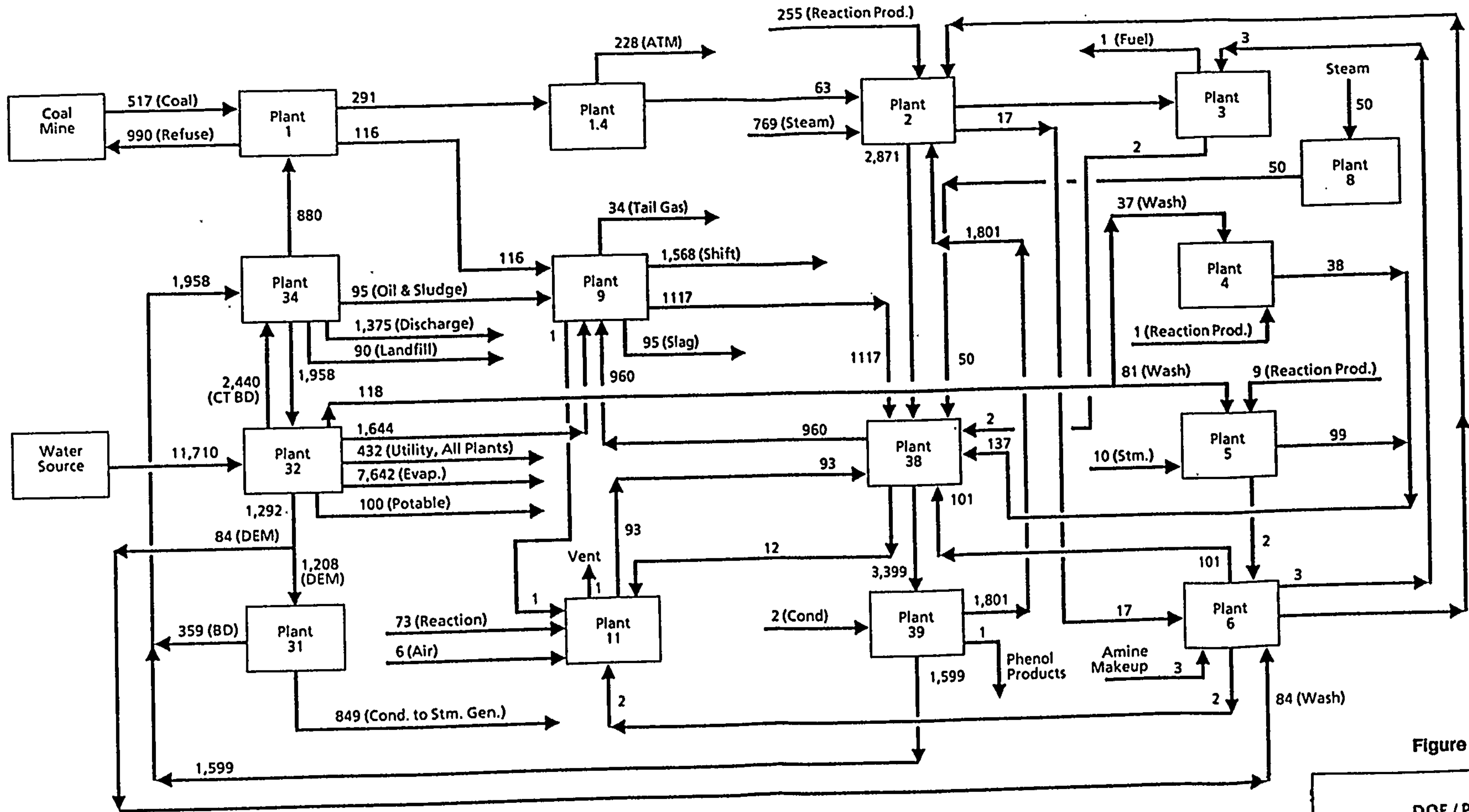


Figure 3.3

NOTES:
Hydrogen flow rates are in MMSCFD (Pure H2)

OVERALL HYDROGEN FLOW DISTRIBUTION

H2FLOCHT.DRW



Notes:

1. Flows are for normal operation and in GPM

Figure 3.4

DOE / PETC
COAL LIQUEFACTION
IMPROVED BASELINE CASE

OVERALL WATER FLOW
DISTRIBUTION

1092048-2

3.3 TASK III

Task III concerns the development of the cost estimate and economics for the base-line design and the alternates for the coal liquefaction facility as well as for the improved baseline design and the option case (option 6) producing hydrogen by natural gas reforming. This part of the study includes the compilation of equipment and utilities summaries, development of scaling factors for equipment sizes and plant costs, and development of the estimates for capital cost, working capital, and owner's costs. Work to perform the economic analyses includes the workup of the manpower requirements and operating costs for the baseline design and for the options and the completion of sensitivity studies.

In this task plants are handled as packaged plants or blocks for the purpose of capital investment, and operating costs as well as overall capacity scale-up.

- During the previous reporting period, March 16, 1992 through June 21, 1992, based on the DOE/PETC/Bechtel/Amoco review meeting of February 24-25, 1992 capital cost estimates for the baseline design as well as all seven options were completed for two different scenarios. These scenarios are for: 1) the First Plant and, 2) Nth plant. Later, the Nth plant concept has been accepted for further economic evaluation. During this reporting period, the capital cost and operating requirements for the improved baseline has been initiated.

- The comments on the draft Topical/Task III report (in 2 volumes) containing capital cost and operating requirements for the baseline and options were obtained from DOE/PETC. During this reporting period, the final version of volumes I and II of the Topical/Task report has been published. Besides incorporation of all comments, the final report contains the updated (fine-tuned) capital costs and operating requirements for all seven options for the "First Plant" and for the "Nth Plant" scenarios.

  The remaining volume (Volume III) of this report containing economics will be completed and issued as a part of the final project report after the improved baseline case is completed.

3.4 TASK IV

Task IV concerns the development of the mathematical algorithms and models for equipment sizing, scale-up, costing, and train duplication for incorporation into the ASPEN/SP process simulation model being developed in Task V.

3.4.1 Status of Task IV

The final topical/task report for Task IV was published in October 1991.

3.5 TASK V

Task V concerns the development of the ASPEN process simulation model of the baseline design. The model will produce complete heat and material balances, elemental balances around each plant and the entire process complex, a major equipment list and outline specifications for Plant 2, utility requirements, capital cost for all plants, and a discounted cash flow economic model for the total complex. The model will be suitable for studying technology advances and options in a case study approach. The model will not include optimization capabilities.

3.5.1 Status of Task V

During this reporting period several accomplishments were made in this task. These accomplishments are listed below.

- The ASPEN computer model had been tuned to match the baseline design. Capital cost changes reflecting recommendation of the DOE/PETC/Bechtel/Amoco February, 1992, review meeting have been integrated.

- The ASPEN based kinetic model is being tuned to match the baseline design. Testing of the model is in progress.

- Completed the final tuning of the kinetic model for the coal liquefaction reactors of Plant 2 to incorporate the recent Wilsonville data.

- The draft of the Topical/Task Report for Task V was issued to DOE/PETC for their comments. This report is in two volumes; Volume I discusses the process simulation model for the baseline design and the seven option cases, and Volume II discusses the LOTUS spreadsheet economic model and the ASPEN/SP kinetic model for coal liquefaction reactors. In addition, the report has a three part Appendix which contains listings of the complete ASPEN/SP input and Fortran files, and detailed documentation for the LOTUS spreadsheet economic model.

- The previously developed kinetic and ebullated bed hydrodynamic models were used to design liquefaction reactor for the higher space velocity case. During the reporting period, optimization of the reactor design was continued. This was to account for (1) internally treated as well as untreated gas recycle rates, (2) recycle solvent composition (3) changes in overall coal conversion and ROSE-SR organic loss and (4) revised gas and liquid yields (relative to the previous baseline design) in the first and second reactor stages. The higher space velocity design case is based on four reactor trains with a coal flowrate of 343,800 lbs of MAF coal per hour per train.

- Economics model based on Lotus 1-2-3 spreadsheets has been revised to incorporate the updated set of key assumptions based on DOE/PETC's input. Revised documentation reflecting these changes has been completed.

- During March 16, 1992 through June 21, 1992 reporting period, a draft of Volume I and Appendix I of the Topical/Task report for Task 5 was completed. Volume I contained documentation for 1) the baseline design and cost estimate model for the "First Plant" case and 2) the Lotus 1-2-3 spreadsheet economic model and 3) how to use it.

3.6 TASK VI

Task 6 concerns the development of a training manual and a training course for the process simulation model. The training course will include an overview of the system, modification of the reporting system, interfacing user models, modification of chemical properties, use of the cost and economics modules, specifying flowsheets, streams, components, properties, and convergence. Trainees will be instructed through the use of case study example problems.

3.6.1 Status of Task VI

- The draft Topical Report for Task VI (training) has been revised and issued. This revision was to reflect DOE's comments and conform to the final version of the models. In addition, this report was split into two volumes; the first volume covers the ASPEN/SP process simulation model, and the second discusses the LOTUS economic model and the kinetic model for the coal liquefaction reactors.

4. KEY PERSONNEL STAFFING REPORT

Key Personnel staffing report for this reporting period (March 16, 1992 through June 21, 1992) as required by DOE/PETC is included in Table 4-1 shown below.

Table 4-1
Key Personnel Staffing Report

Duration of Quarter From June 22, 1992 through September 13, 1992

Name of Key Person	Function	% Time Spent*
Bechtel:		
S. N. Habash[1]	Project Manager	3
S. K. Poddar	Project Manager	34
S. K. Poddar	Process Manager	50
T. J. Reynolds	Project Secretary	39
Amoco:		
A. B. Schachtschneider	Project Manager	10
S. J. Kramer	Principal Investigator	65
A. Basu	Principal Investigator	15

* (Number of hours spent/total available working hours for June 22, 1992 through September 13, 1992) x 100.

1 S. K. Poddar was assigned to the Project Manager position replacing S. N. Habash at the end of June, 1992.